Absence of Coexistence of Superconductivity and Antiferromagnetism of the Hole-Doped Two-Dimensional Extended $t-J$ Model

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The possibility of coexistence of superconductivity (SC) and antiferromagnetic long range order (AFLRO) of the two-dimensional extended $t-J$ model in the very underdoped region is studied by the variational Monte-Carlo (VMC) method. In addition to using previously studied wave functions, a recently proposed new wave function generated from the half-filled Mott insulator is used. For hole-doped systems, the phase boundary between AFLRO and $d-$wave SC for the physical parameters, $J/t = 0.3$, $t'/t = -0.3$ and $t''/t = 0.2$, is located near hole density $\delta_c = 0.06$, and there is *no* coexistence. The phase transition is first-order between these two homogeneous phases at δ_c.

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Correlation between the d-wave SC and AFLRO is one of the critical issues in the physics of the high-temperature superconductivity (HTS)[1, 2]. Early experimental results showed one of the common features of the HTS cuprates is the existence of AFLRO at temperature lower than the Néel temperature T_N in the insulating perovskite parent compounds. When charge carriers (electrons or holes) are doped into the parent compounds, AFLRO is destroyed quickly and then SC appears. In most thermodynamic measurements, AFLRO does not coexist with SC[3]. However, this is still a controversial issue. Recent experiments such as neutron-scattering and muon spin rotation show that the spin density wave (SDW) may compete, or coexist with SC under the external magnetic field [4, 5, 6]. Remarkably, elastic neutron scattering experiments for underdoped $YBa_2Cu_3O_x$ ($x = 6.5$ and 6.6, $T_c = 55K$ and $62.7K$, respectively) show that the commensurate AFLRO develops around room temperature with a large correlation length $\sim 100\mathring{A}$ and a small staggered magnetization $m_0 \sim 0.05\mu_B$[7, 8, 9]. These results suggest that AFLRO may coexist with SC but the possibility of inhomogeneous phases is not completely ruled out.

For the theoretical part, the two-dimensional (2D) t-J model is the first model proposed[10] to understand the physics of HTS. Anderson proposed the resonating-valence-bond (RVB) theory for the model about one and a half decades ago. The theory is reexamined again[11] recently. The authors compared the prediction of the RVB theory with several experimental results and found the theory to have successfully explained the main features of cuprates. This so called "plain vanilla" theory did not consider the issue of AFLRO, which must be addressed at very low doping. From analytical and numerical studies of the $t-J$ model, it was shown that at half-filling, the $d-$wave RVB state with AFLRO is a good trial wave function (TWF). In this case, SC correlation is zero because of the constraint of no-double-occupancy. Upon doping, the carriers become mobile and SC revives while AFLRO is quickly suppressed. However, if the doping density is still small, AFLRO will survive. Thus SC and AFLRO coexist in the very underdoped regime[12, 13, 14, 15, 16]. Exact diagonalization (ED) up to 26 sites show that both SC and AFLRO are enhanced by the external staggered field. This result also implies these two orders can coexist homogeneously in a 2D $t-J$ model[17]. However, the regime of AFLRO predicted by these studies extend to larger doping than the experimental results. The robustness of the coexistence of SC and AFLRO seems to be inconsistent with experiments[18].

There are several experimental and theoretical studies suggesting the presence of the next- and third-nearest-neighbor hopping terms t' and t'' in cuprates. For example, the topology of the large Fermi surface and the single-hole dispersion studied by ARPES [19], and the asymmetry of phase diagrams of the electron- and hole-doped cuprates can be understood by introducing these terms. Further, these longer range hopping terms may be essential for the large enough T_c for the $t-J-$type models[20, 21]. In this paper, we'd like to demonstrate the phase diagram constructed by VMC results of the extended $t-J$ model. The trial WF's for very underdoped systems are generalized from the single-hole and slightly-doped WF proposed by Lee *et al.*[22, 23]. The results for the hole-doped case show there is *no* coexistence of $d-$wave pairing and AFLRO when the next- and third-nearest neighbor hopping terms are introduced. And the

phase boundary of AFLRO is pushed to lower doping density.

The Hamiltonian of the extended $t-J$ model is

$$H = H_t + H_J = \quad (1)$$
$$-\sum_{ij} t_{ij}(\tilde{c}^\dagger_{i,\sigma}\tilde{c}_{j,\sigma} + H.C.) + J\sum_{<i,j>}(\mathbf{S_i}\cdot\mathbf{S_j} + \frac{1}{4}n_i n_j)$$

where $t_{ij} = t$, t', and t'' for sites i and j are nearest, next nearest, and the third nearest neighbors. $< i,j >$ in H_J means the spin-spin interaction occurs only for nearest neighbors. $\tilde{c}_{i,\sigma} = (1-n_{i,-\sigma})c_{i,\sigma}$, satisfies the no-double-occupancy constraint. At half-filling, the system is reduced to the Heisenberg Hamiltonian H_J. As carriers are doped into the parent compound, H_t is included in the Hamiltonian.

First we exam the phase diagram of the $t-J$ model, that is, $t' = t'' = 0$. Following Ref.[15, 22], three mean-field order parameters are introduced: the staggered magnetization $m_s = \langle S^z_A\rangle = -\langle S^z_B\rangle$, where the lattice is divided into A and B sublattices, the uniform bond order parameters $\chi = \langle\sum_\sigma c^\dagger_{i\sigma}c_{j\sigma}\rangle$, and $d-$wave RVB ($d-$RVB) one $\Delta = \langle c_{j\downarrow}c_{i\uparrow} - c_{j\uparrow}c_{i\downarrow}\rangle$ if i and j are n.n. sites in the x direction and $-\Delta$ for the y direction. The Lee-Shih WF, which is the mean-field ground state WF is

$$\mid \Psi_{LS}\rangle = P_d\left(\sum_{\mathbf{k}\in SBZ}(A_\mathbf{k}a^\dagger_{\mathbf{k}\uparrow}a^\dagger_{-\mathbf{k}\downarrow} + B_\mathbf{k}b^\dagger_{\mathbf{k}\uparrow}b^\dagger_{-\mathbf{k}\downarrow})\right)^{N_s/2}\mid 0\rangle \quad (2)$$

where N_s is the total number of sites and $A_\mathbf{k} = (E^{(1)}_\mathbf{k} + \xi^-_\mathbf{k})/\Delta_\mathbf{k}$ and $B_\mathbf{k} = -(E^{(2)}_\mathbf{k} - \xi^+_\mathbf{k})/\Delta_\mathbf{k}$ with $E^{(1)}_\mathbf{k} = (\xi^{-2}_\mathbf{k} + \Delta^2_\mathbf{k})^{1/2}$ and $E^{(2)}_\mathbf{k} = (\xi^{+2}_\mathbf{k} + \Delta^2_\mathbf{k})^{1/2}$. Here $\Delta_\mathbf{k} = \frac{3}{4}\Delta(cosk_x - cosk_y)$. Energy dispersions for the two SDW bands are $\xi^\pm_\mathbf{k} = \pm[(\epsilon_\mathbf{k}+\mu)^2 + (Jm_s)^2]^{1/2} - \mu$ with $\epsilon_\mathbf{k} = -2(t\delta + \frac{3}{8}J\chi)(cosk_x + cosk_y)$. $a_{\mathbf{k}\sigma} = \alpha_\mathbf{k}c_{\mathbf{k}\sigma} + \sigma\beta_\mathbf{k}c_{\mathbf{k}+\mathbf{Q}\sigma}$ and $b_{\mathbf{k}\sigma} = -\sigma\beta_\mathbf{k}c_{\mathbf{k}\sigma} + \alpha_\mathbf{k}c_{\mathbf{k}+\mathbf{Q}\sigma}$, where $\mathbf{Q} = (\pi,\pi)$, $\alpha^2_\mathbf{k} = \frac{1}{2}\{1 - [(\epsilon_\mathbf{k}+\mu)/(\xi^+_\mathbf{k}+\mu)]\}$ and $\beta^2_\mathbf{k} = \frac{1}{2}\{1 + [(\epsilon_\mathbf{k}+\mu)/(\xi^+_\mathbf{k}+\mu)]\}$, are the operators of the lower and upper SDW bands, respectively. μ is the chemical potential which determines the number of electrons. Note that the summation in Eq.(2) is taken over the sublattice Brillouin zone (SBZ). The operator P_d enforces the constraint of no doubly occupied sites for cases with finite doping.

For the half filled case, $\mu = 0$ and the optimal variational energy of this TWF obtained by tuning Δ and m_s in the VMC simulation is $-0.332J$ per bond which is within 1% of the best estimate of the ground state energy of the Heisenberg model. For the case of pure AFLRO without Δ, energy per bond is about 3 to 4% higher. Upon doping, there are two methods to modify the TWF: one is to use the SDW bands with a nonzero μ, the other is to create charge excitations from the half-filled ground states. For the former method, the TWF is optimized by tuning Δ, m_s and μ. Note that for larger doping densities, AFLRO disappears ($m_s = 0$) and the WF reduces to the standard $d-RVB$ WF. For the latter method, the WF is the "small Fermi pocket" state $\mid \Psi_p\rangle$:

$$\mid \Psi_p\rangle = P_d\left(\sum_{\mathbf{k}\in SBZ,\mathbf{k}\notin Q_p}(A_\mathbf{k}a^\dagger_{\mathbf{k}\uparrow}a^\dagger_{-\mathbf{k}\downarrow} + B_\mathbf{k}b^\dagger_{\mathbf{k}\uparrow}b^\dagger_{-\mathbf{k}\downarrow})\right)^{N_s/2}\mid 0\rangle \quad (3)$$

$\mathbf{k}\notin Q_p$ means the $\mathbf{k}$ points in the Fermi pocket Q_p are not occupied. For example, for 4 holes in 12×12 lattice, $Q_p = \{(\pi/2,\pi/2),(\pi/2,-\pi/2)\}$. The number of holes is twice of the number of $\mathbf{k}$-points in Q_p and μ is identical to zero in Eq.(3). In general, for the ground state the set Q_p should be determined variationally. Yet as we expect, it agrees well with the rigid band picture in the slightly doped cases as in Ref.[23].

The staggered magnetization $\langle M\rangle = \frac{1}{N_s}\langle\sum_j e^{i\mathbf{Q}\cdot\mathbf{R_j}}S^z_{\mathbf{R_j}}\rangle$ and the d-wave pair-pair correlation $P_d(\mathbf{R}) = \frac{1}{N_s}\langle\sum_i \Delta^\dagger_{\mathbf{R_i}}\Delta_{\mathbf{R_i}+\mathbf{R}}\rangle$, where $\Delta_{\mathbf{R_i}} = c_{\mathbf{R_i}\uparrow}(c_{\mathbf{R_i}+\hat{\mathbf{x}}\downarrow} + c_{\mathbf{R_i}-\hat{\mathbf{x}}\downarrow} - c_{\mathbf{R_i}+\hat{\mathbf{y}}\downarrow} - c_{\mathbf{R_i}-\hat{\mathbf{y}}\downarrow})$ are measured for $J/t = 0.3$ and $t' = t'' = 0$ for the 12×12 lattice with periodic boundary condition. P^{ave}_d is the averaged value of the long-range part ($\mid \mathbf{R} \mid > 2$) of $P_d(\mathbf{R})$. The resulting $\langle M\rangle$ (full circles) and P^{ave}_d (empty circles) are shown in Fig.1.

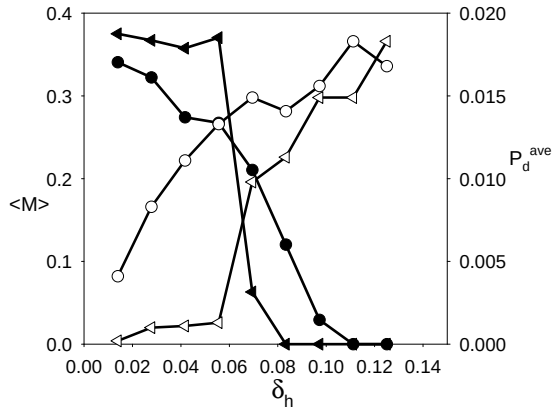

FIG. 1: $\langle M\rangle$ (full symbols) and P^{ave}_d (empty symbols) for $J/t = 0.3$, $t' = t'' = 0$ (circles) and $t'/t = -0.3$, $t''/t = 0.2$ (triangles) for hole doped 12×12 lattice.

It can be seen in Fig.1 that in the underdoped region for the $J/t = 0.3$, $t' = t'' = 0$ case, AFLRO (full circles) coexists with SC (open circles) for $\delta_c \leq 10\%$, which is smaller than the weak-coupling mean-field result $\sim 15\%$[15], but still larger than the phase boundary of AFLRO determined by experiments $\delta_c < 5\%$. The energies of $\mid \Psi_{LS}\rangle$ are lower than those of $\mid \Psi_P\rangle$ for all doping densities in this case. This result is also consistent with the results reported by Himeda and Ogata[16]. The VMC result is more realistic than the weak-coupling one. It may result from the rigorous no-double-occupancy constraint that suppresses the AFLRO faster than the

constraint-relaxed mean-field approximation.

Now we examine the phase diagram for $J/t = 0.3$, $t'/t = -0.3$ and $t''/t = 0.2$. For this case, the WF Eq.(2) is modified by replacing μ by $\mu + 4t'_v cosk_x cosk_y + 2t''_v(cos2k_x + cos2k_y)$ due to the second and third nearest neighbor hopping terms. t'_v and t''_v are variational parameters. t'_v and t''_v are not necessarily equal to the bare values t' and t'' because the constraint strongly renormalizes the hopping amplitude. On the other hand, the effect of t' and t'' on $\mid \Psi_P\rangle$ is the choice of **k**-points in Q_p, and the form of Eq.(3) is not changed.

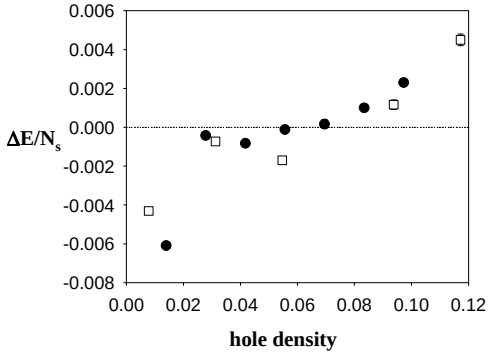

FIG. 2: Energy difference per site between the two wave functions $\mid \Psi_P\rangle$ and $\mid \Psi_{LS}\rangle$ for $t'/t = -0.3$ and $t''/t = 0.2$ in 12×12 (full circles) and 16×16 (open squares) lattices.

The optimal wave functions for different densities are determined by minimizing the variational energies among $\mid \Psi_p(m_s, \Delta, \{Q_p\})\rangle$ and $\mid \Psi_{LS}(m_s, \Delta, t'_v, t''_v, \mu)\rangle$. The differences of the energies of best $\mid \Psi_P\rangle$ and $\mid \Psi_{LS}\rangle$ for various hole densities are shown in Fig.2. $\langle M\rangle$ (full triangles) and P_d^{ave} (open triangles) for 12×12 lattice are shown in Fig.1.

It can be seen that level crossing occurs at $\delta_h \sim 0.06$. $\mid \Psi_P\rangle$ has lower energy below the critical density. To show $\mid \Psi_{LS}\rangle$ and $\mid \Psi_p\rangle$ belong to two different types of WF, we calculate the overlap of them. $(\frac{\langle \Psi_{LS}|\Psi_p\rangle}{|\Psi_{LS}||\Psi_p|})$ is only 0.0113(4). The almost orthogonality of the two wave functions implies that the ground state WF's switch at the critical density. Another evidence is shown by the correlation functions of the two wave functions shown in Fig.3. It is clear that the holes in $\mid \Psi_p\rangle$ repel each others and pairing is very small, while the behavior is opposite for $\mid \Psi_{LS}\rangle$.

For $\delta_h < 0.06$, $\mid \Psi_p\rangle$ is the ground state WF and $\langle M\rangle$ is a little larger than the $t' = t'' = 0$ case while P_d^{ave} is suppressed by one order of magnitude. Thus there is AFLRO but *no* SC in this regime. The behavior is quite different from $\mid \Psi_{LS}\rangle$ for the same doping regime for $t' = t'' = 0$ case, whose P_d^{ave} coexists with $\langle M\rangle$. The possible reason is that the WF $\mid \Psi_p\rangle$ gains energy (short-range effect) from its $d - RVB$ feature as $\mid \Psi_{LS}\rangle$, yet P_d^{ave} is greatly suppressed by replacing μ by Q_p to control the density. This replacement seems to make the WF decoherent for pairing.

For δ_h larger than 0.06, the RVB state ($m_s = 0$ in $\mid \Psi_{LS}\rangle$) optimizes the energy. P_d^{ave} increases and $\langle M\rangle$ drops to zero sharply. Unlike the $t' = t'' = 0$ case there is no region optimized by $\mid \Psi_{LS}\rangle$ with non-zero m_s. In conclusion, there is no coexistence of AFLRO and SC for the $t'/t = -0.3, t''/t = 0.2$ case. These parameters are close to the values for YBCO and BSCO compounds[24].

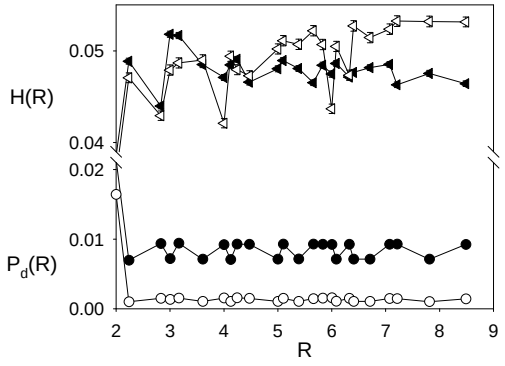

FIG. 3: Pair-pair correlation $P_d(R)$ (circles) and hole-hole correlation $H(R)$ (triangles) of $\mid \Psi_{LS}\rangle$ (full symbols) and $\mid \Psi_p\rangle$ (open symbols) for 8 holes in a 12×12 lattice.

In summary, for the extended $t-J$ model, we proposed a new WF $\mid \Psi_p\rangle$ for the underdoped regime which has lower variational energy than the traditional WF with coexisting AFLRO and SC. This WF is constructed under the framework of RVB. The new wave function has AFLRO but SC is largely suppressed and there is no coexistence of AFLRO and SC in the underdoped regime of the hole-doped extended $t-J$ model. The variational phase diagram shows better agreement with experimental results for the underdoped HTS cuprates.

Note that in this study we only consider the homogeneous states. Since the phase transition comes from the level crossing of the two classes of states at the critical density $\delta_c = 0.06$, it is a first order phase transition. It is quite natural to have inhomogeneity in the system near the critical point[25]. It may also lead to other more novel inhomogeneous states such as stripe phase[26]. Another interesting result of our study is that the non-coexistence of SC and AFLRO is much more robust for systems with larger values of t'/t and t''/t such as YBCO and BSCO[24]. For LSCO where t'/t and t''/t are smaller, the tendency toward coexistence is larger and the possibility of inhomogeneous phase will become much more likely.

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